

Acetic acid

64-19-7 | DTXSID5024394

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 14.1 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.48e-01

Confidence level: 7.34e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Acetic acid</div> <div>Measured: 16.7</div> <div>Predicted: 14.1</div>	<div>Image not found</div> <div>Acrylic acid</div> <div>Measured: 13.9</div> <div>Predicted: 9.22</div>	<div>Image not found</div> <div>Propionic acid</div> <div>Measured: 13.5</div> <div>Predicted: 6.36</div>
<div>Image not found</div> <div>Sodium propionate</div> <div>Measured: 5.20</div> <div>Predicted: 6.36</div>	<div>Image not found</div> <div>Formic acid</div> <div>Measured: 21.7</div> <div>Predicted: 10.9</div>	